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Evolution of Co charge disproportionation with Na order in NaxCoO2

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Abstract

© 2014 American Physical Society. Co59NMR experiments have been performed on single crystals of the layered cobaltate NaxCoO2with x=0.77, which is an antiferromagnet with Néel temperature TN=22 K. In this metallic phase, six Co sites are resolved in the NMR spectra, with distinct quadrupole frequencies νQ, magnetic shifts KZZ and nuclear spin lattice relaxation rates 1/T1. Contrary to the x=1/2 or x=2/3 phases, the 3D stacking of the Na planes is not perfect for x=0.77 but this does not influence markedly the electronic properties. We evidence that the magnetic and charge properties of the Co sites are highly correlated with each other as KZZ and (1/T1)1/2 scale linearly with νQ. The data analysis allows us to separate the contribution νQlatt of the ionic charges to νQ from that νQel due to the hole orbitals on the Co sites. We could extend coherently this analysis to all the known phases in the Na cobaltate phase diagram. The variation with x of νQlatt is found to fit rather well numerical computations done in a point charge model. The second term νQel allowed us to deduce the hole concentration on the cobalts. These detailed experimental results should stimulate theoretical calculations of the electronic structure involving both the Co orbital configurations and DMFT approaches to take into account the electronic correlations.

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